APPLICATION OF EXPERIMENTAL DESIGN THEORY TO OCEAN REMOTE SENSING WITH A HYPERSPECTRAL DETECTOR*

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ABSTRACT

A method based on a theory of experimental Optimal Design (OD) was developed in Russia to select the best combination of wavelengths so an optically remote spectral sensor may optimally estimate oceanic chlorophyll concentration. It gives the number of spectral bands, their center wavelength, and each band's spectral width to make the best estimate of chlorophyll concentration in a fixed observation time. A hyperspectral sensor is convenient because it eliminates the need for variable optical filters. An ideal sensor would have an infinite number of infinitesimally narrow spectral bands. Optimal designs are given for both ideal and real sensors. The designs were computed using ocean radiance spectra simulated by a Monte Carlo model for a range of chlorophyll concentrations. The computed OD was tested for robustness over a wide range of experimental conditions. The methods of color index and principal component analysis were also applied. The optimal design method gives more accurate chlorophyll estimates.

1.0 INTRODUCTION

An important task for the modern remote sensing oceanographer is the accurate estimate of in situ chlorophyll (or other in situ parameters) from spectral measurements of water leaving radiance. A method was developed (Kozlov, *et al.*, 1992, Levin, *et al.*, 1994, 1996, and 1997, and Zolotukhin, *et al.*, 1997) to optimally select spectral channels for the remote determination of an in situ ocean parameter. This method was based on a theory of Experimental Design originally suggested by V. Kozlov, (1974 and 1983). It has a few advantages over the present methods of color index and principal component analysis used for chlorophyll estimation. The wavelengths considered in these latter methods are often qualitatively selected and, thus, do not guarantee an optimal use of spectral channels. Spectral bands generally have the same width, e.g., 5, 10, or 20 nm, with the result that optimal spectral width is not treated. Additionally, noise found in real sensor data is not addressed. In contrast, the Optimal Design (OD) algorithm searches for the truly optimal spectral channels, giving center wavelengths and band widths while accounting for thermal and shot noise (Levin, *et al.*, 1994, 1997, and Kozlov, *et al.*,1989).

The OD algorithm uses as input the first two moments of the joint distribution of remotely measured ocean radiance spectra $u(\lambda)$ and the parameter of interest Θ (here, chlorophyll concentration). The spectra $u(\lambda)$ are expressed as the number of primary electrons in each of the sensor's spectral bands per unit time. As noted, the parameter Θ may be the concentration of phytoplankton, sediment or some other optically active matter. The moments of the distribution $(u(\lambda), \Theta)$ are: $\langle\Theta\rangle$ and σ^2, the mean and variance of Θ; $f(\lambda) = \langle u(\lambda)\rangle$, the mean value of observed spectral photoelectrons $u(\lambda)$; $K(\lambda,\lambda') = \mathrm{cov}\,(u(\lambda), u(\lambda'))$, the auto-covariance function of $u(\lambda)$; and $q(\lambda) = \mathrm{cov}\,(u(\lambda), \Theta)$, the covariance between $u(\lambda)$ and Θ.

Given the statistics on $(u(\lambda), \Theta)$, an optimal design ξ may be computed which determines the number of independent channels r of the sensor, the spectral transmittance function $x_i(\lambda)$ for each channel, and the time periods allotted for measurements in each channel. The t_i are constrained by $\Sigma t_i = t$, i.e., the overall observation time is fixed. Since $x_i(\lambda)$ is the spectral transmittance function of the i-th channel, then $0 < x_i(\lambda) < 1$. Each channel may consist of multiple spectral bands. The signal observed by the optimally selected filter $x_i(\lambda)$ is represented as y_i, the number of primary electrons in the i-th channel in the time period t_i.

* Presented at the Fifth International Conference on Remote Sensing for Marine and Coastal Environments, San Diego, California, 5-7 October 1998.

Kozlov, *et al.*, (1989) showed that the best linear estimate $\hat{\Theta}$ of the parameter Θ is given by

$$\hat{\Theta} = \langle\Theta\rangle + q^T D^{-1} T^{-1} Y, \tag{1}$$

with the residual variance of this estimate, considered to be a measure of design optimality or "goodness," given as

$$h(\xi) = \sigma^2 - q^T D^{-1} q, \tag{2}$$

where $q = (q_1,...q_r)^T$, $q_i = \int q(\lambda)x_i(\lambda)d\lambda$, $D = K + \mathrm{diag}(f_i + v)T^{-1}$, $K = \|K_{ij}\|_{i,j=1}^r$, $Kij = \iint K(\lambda,\lambda')x_i(\lambda)x_j(\lambda)d\lambda d\lambda'$, $f_i = \int f(\lambda)x_i(\lambda)d\lambda$, $T = \mathrm{diag}(t_i)$, $Y = (y_1,...y_r)^T$, and v is the noise, independent of the signal level. They also proved that the optimal design consists of no more than two spectral channels ($r = 2$), taking on values of only 0 or 1, i.e., there will be only two filters, $x_1(\lambda)$ and $x_2(\lambda)$, each consisting of a number of rectangular transmission bands.

The algorithm was originally used by Levin (1996, 1997) and Zolotuchin (1997) to estimate chlorophyll concentration C in the ocean for a sensor with a photomultiplier and a spectral filter device which allocated the measurement time t between two spectral channels $x_1(\lambda)$ and $x_2(\lambda)$ into periods t_1 and t_2 respectively. The spectrometer SFS-1 (Afonin, *et al.*, 1987), with a rotating filter set, is such a sensor; sequentially sampling different spectral bands.

In this paper, we apply the OD theory to the problem of ocean remote sensing with a hyperspectral sensor system, which eliminates the need for variable optical filters. Accordingly, noise is considered that of a semi-conductor detector, and radiation is received simultaneously by both channels over the entire measurement time, corresponding to the condition $t_1 = t_2 = 0.5t$, where t is the total measurement time used in the OD calculation, not the sensor frame time (which is actually t_1 or t_2). The spectral width of the hyperspectral sensor, although small, is finite, thus imposing a limit on the realization of an "ideal" optimal design.

2.0 SIMULATION OF INPUT RADIANCE SPECTRA

The OD method requires the use of a large database of upwelled radiance spectra related to in situ chlorophyll. The collection of such a database is prohibitively expensive. Thus the approach taken was to simulate the spectra for the database using a Monte Carlo oceanic radiance model. Atmospheric light and scattering were made negligible by only modeling the data that would be obtained from shipboard or low-flying airborne observations.

The OD method uses the joint distribution statistic ($u(\lambda)$, C) for spectral photoelectrons and chlorophyll. The spectrum $u(\lambda)$, the spectral density of the primary electrons per unit time (e.g., [μ^{-1} s^{-1}]), is obtained using the radiance spectral density $L_t(\lambda)$. $L_t(\lambda)$ is the sum of spectral densities of the water-leaving radiance just above the surface, $L'(\lambda)$, and of the radiance reflected from the sea surface, $L_s(\lambda)$, with units of [W m^{-2} sr^{-1} μ^{-1})]. Thus

$$u(\lambda) = L_t(\lambda)\, A\, \tau(\lambda)\, \omega\, \eta(\lambda) e^{-1}(\lambda), \tag{3}$$

$$L_t(\lambda) = L'(\lambda) + L_s(\lambda), \tag{3a}$$

where A [m^2], $\tau(\lambda)$, ω [sr], and $\eta(\lambda)$ are the sensor parameters, i.e., aperture (entrance pupil) area, transmittance, receiver solid angle, and photo-detector quantum efficiency (QE). $e(\lambda)$ is the photon energy (e [J] $\cong 2\text{x}10^{19}/\lambda$ [μ]). L' is related to the reflectivity coefficient $\rho = \pi L/E_d$ (L is the spectral density of the water-leaving radiance just beneath the sea surface) as

$$L'(\lambda) = c_s \pi^{-1} \rho(\lambda) E(\lambda), \tag{4}$$

where $E(\lambda)$ [W m^{-2} μ^{-1}] is the spectral density of solar irradiance of the sea surface and $c_s = 0.533$ (Austin, 1974) takes into account the radiance change through the water-air interface. The sea surface radiance $L_s(\lambda)$ for a rough surface is obtained from $\rho_s(\lambda) = \pi L_s(\lambda)/E(\lambda)$. Substituting for $L(\lambda)$ and $L_s(\lambda)$, $L_t(\lambda)$ is given as

$$L_t(\lambda) = \pi^{-1} E(\lambda)\ [0.533\rho(\lambda) + \rho_s(\lambda)]\,. \tag{5}$$

We consider only a cloudless sky. The irradiance $E(\lambda)$ is a sum of irradiances from direct sunlight $E^{dir}(\lambda)$ and from diffusive sky light, $E^{dif}(\lambda)$, assumed to be uniform. For each irradiance, water leaving and surface reflected, the corresponding coefficients take the different values (ρ^{dir}, ρ_s^{dir}) and (ρ^{dif}, ρ_s^{dif}). In the general case,

$$\rho = \alpha\rho^{dir} + (1-\alpha)\rho^{dif},\ \ \rho_s = \alpha\rho_s^{dir} + (1-\alpha)\rho_s^{dif}, \tag{6}$$

where α is the ratio of direct sunlight to the total sea surface irradiance.

The coefficients ρ_s^{dir} were computed for nadir viewing direction by Mullamaa's formula based on the Cox-Munk surface slope distribution (Mullamaa, 1964). They are functions of wind velocity v, azimuth angle φ_v, and solar zenith angle θ_0. Table 1 shows several examples of calculated values of ρ_s^{dir}. For a uniform sky in nadir direction, $\rho_s^{dif} \approx 0.02$ is virtually independent of wind velocity (Mullamaa, 1964).

Table 1. Surface Radiance Coefficients

The values of surface radiance coefficients ρ_s^{dir} (averaged over azimuth φ_v) for direct sunlight in the nadir viewing direction					
Solar zenith Angle $\theta°$	Wind velocity v (m/s) 2	5	10	15	20
0	0.42	0.20	0.10	0.072	0.054
20	0.036	0.064	0.061	0.051	0.043
45	0.0001	0.0016	0.008	0.014	0.018

The coefficients ρ^{dir} and ρ^{dif} for nadir viewing, accounting for particle and molecular scattering, were calculated (Levin, 1997) as:

$$\rho^{dir} = \frac{1-\eta_w + 0.8(1+0.8\mu_0^2)\eta_w}{2(1+\mu_0)} \frac{b_b}{a+b_b}, \tag{7}$$

$$\rho^{dif} = (0.27 + 0.07\eta_w)\, b_b/(a+b_b), \tag{8}$$

where a and b_b are the absorption and backscattering coefficients, $\mu_0 = \cos[\arcsin(\sin\theta_0/n)]$, $\eta_w = b_{bw}/b_b$, and b_{bw} is the backscattering coefficient of optically pure water. $a(\lambda)$ and $b_b(\lambda)$ were obtained as functions of concentrations of chlorophyll (C), yellow substance (Y) and sediment particles (X) through the use of the models of Prieur and Sathyendranath (1981) and Sathyendranath, *et al.* (1989). Following Sathyendranath, *et al.* (1989), the ranges of C, X and Y were selected to be $C = 0.01 - 100$ mg m^{-3}, $X = 0.01 - 10$ m^{-1}, and $Y = 0.01 - 1$ m^{-1}.

One thousand water samples of varying C, X, and Y were chosen for Monte Carlo modeling by randomly sampling the above-mentioned C, X, and Y distributions. The logarithm of each concentration was assumed to be uniformly distributed over the range given above. The solar angle θ_0 was distributed uniformly within the limits of 40-60° (at smaller solar angles the amount of sun glint in the receiver view increased sharply). The wind velocity v followed a Rayleigh distribution with mean velocity <v> = 10 m/s, and the azimuthal angle φ_v was uniform within the limits of 0-180°. The solar irradiance density $E(\lambda)$ for various θ_0 was taken from tables (Shifrin, *et al.*, 1959), and the ratio $\alpha(\theta_0, \lambda)$ from experimental data (Austin, 1979).

For each combination X, Y, C, θ_0, v and φ_v, the spectra $L_t(\lambda)$ were computed using Eqs. 5-8 and the IOP model of Prieur and Sathyendranath (1981) and Sathyendranath, *et al.*, (1989). A database containing 1000 simulated radiance spectra $L_t(\lambda)$ with a step of 5 nm was obtained.

3.0 THE SENSOR PARAMETERS

Since the OD is calculated from the photoelectron counts in the sensor detector elements, sensor parameters, including noise, that affect the photoelectron count must be taken into consideration. The computations were conducted for a hyperspectral sensor with aperture area $A = 5.7\ 10^{-4}\text{m}^2$ (lens diameter 2.7 cm), field-of-view $\omega = (2\tan\beta/N)^{-2} = 2.4\text{x}10^{-7}$ ($2\beta = 8.94°$ is a total viewing angle over all 320 sensor elements), t = 10.5 ms, QE = 0.6.

A sampling of the other sensor parameters required for the OD computations that vary with spectral detector site is given in Table 2. This table gives the detector spectral channel number (No), the center wavelength λ of that channel in nm, the bandwidth $\Delta\lambda$ of the channel in nm, the total transmittance τ of all the optics and detector coatings, the gain g of the channel in photon-to-electron conversion units, and the signal independent noise ν in number of electrons. The latter includes shot noise of the thermal background radiation, digitizer noise, electronic readout noise, and offset correction error. Parameters presented in Table 2 are typical of a hyperspectral sensor with an InSb detector array. In addition, there is a gain noise factor F = 1.3 that is the same for all elements.

Table 2. The Sensor Parameters

No	λ	$\Delta\lambda$	τ	g	ν	No	λ	$\Delta\lambda$	τ	g	ν
1	400.610	3.07	0.39	1.95	1919	28	507.781	4.94	0.56	1.79	1886
2	403.906	3.11	0.39	1.97	1899	29	512.89	5.04	0.55	1.76	1877
3	407.229	3.15	0.41	1.97	1905	30	518.119	5.16	0.56	1.74	1882
4	410.582	3.20	0.42	1.99	1899	31	523.472	5.28	0.56	1.70	1881
5	413.967	3.24	0.43	1.99	1901	32	528.953	5.4	0.56	1.67	1881
6	417.388	3.28	0.44	2.01	1902	33	534.588	5.53	0.56	1.63	1876
7	420.847	3.34	0.44	2.01	1900	34	540.323	5.58	0.56	1.61	1862
8	424.348	3.39	0.44	2.03	1896	35	546.222	5.8	0.57	1.56	1872
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
25	493.121	4.62	0.55	1.87	1882	52	674.06	8.88	0.59	1.46	1864
26	497.901	4.73	0.55	1.85	1883	53	683.511	9.1	0.59	1.46	1867
27	502.785	4.82	0.56	1.81	1880	54	693.204	9.33	0.59	1.44	1874

4.0 THE OPTIMAL DESIGN

The simulated spectra $L_t(\lambda)$ and the sensor parameters noted above were substituted into Eq. 3 to calculate the distribution of spectral photoelectrons, $u(\lambda)$. The appropriate statistical moments – $<C>$, $f(\lambda)$, $K(\lambda,\lambda')$, and $q(\lambda)$ – were then computed. Then the method noted earlier (Kozlov, *et al.*, 1992, Levin, *et al.*, 1994, 1996, and 1997, and Zolotukhin, *et al.*, 1997) was used to compute the "ideal" OD for a sensor with infinitesimal bands sharing measurement time between two filter configurations. All other sensor parameters (A, ω, $\tau(\lambda)$, η, t, g, ν, and F) used were those of the real sensor. Detector shot noise was computed by multiplying the square root of the number of signal electrons by the gain g and the noise factor F. The resulting Optimal Design for this ideal sensor is as follows: The first combination of spectral bands, for the spectral transmittance function $x_1(\lambda)$, was 400-403, 533-548, 586-614, and 686-700 nm. The second combination, for $x_2(\lambda)$, was 440-459, 548-586, and 660-667 nm. The optimal time of measurement in the first channel was $t_1 = 0.46t$; in the second one $t_2 = 0.54t$.

A best estimate of the chlorophyll concentration C is given by

$$\log C = A_0 + A_1 y_1 - A_2 y_2. \tag{9}$$

where y_1 and y_2 are the signals measured in the two channels $x_1(\lambda)$ and $x_2(\lambda)$, expressed in number of primary electrons. The coefficients A_0, A_1 and A_2, which are calculated by the OD method through Eq. 1, depend only on the product of the sensor and measurement parameters $A\,\omega\,t = M$, but not on the values of the individual parameters. The value of M used in the calculations corresponded to the sensor defined in section 3.0 and gave coefficient values of $A_0 = 0.012$, $A_1 = 3.66\text{x}10^{-2}$ and $A_2 = 6.46\text{x}10^{-2}$. For other sensors with different values of M, Eq. 1 must be used again to calculate the coefficients A_0, A_1 and A_2. The "goodness" of the estimate, $h(\xi) = 0.0099$, i.e., the variance of estimate log C, is calculated using Eq. 2. This variance calculation came from averages over the entire set of chlorophyll cases simulated.

Optimal Design for the real sensor differs from that for the computed ideal sensor. Here the measurement times are equal, $t_1 = t_2$, and the sensor bands are of finite width, varying with wavelength. Therefore, the real sensor OD closest to the ideal uses the spectral band weights for the first and the second channels shown in Tables 3a and 3b respectively. The signals from the sensor bands in the first line of the tables are to be multiplied by the corresponding weights in the second line of the tables.

Table 3a. Weights for Channel 1

Sensor band	1	33	34	35	42	43	44	45	54
Signal weight	1.0	0.69	1.0	0.87	1.0	1.0	1.0	0.50	1.0

Table 3b. Weights for Channel 2

Sensor band	13	14	15	16	17	36	37	38	39	40	41	51
Signal weight	1.0	1.0	1.0	1.0	0.72	1.0	1.0	1.0	1.0	1.0	0.64	1.0

For the real sensor, the Optimal Design gives the coefficients $A_0 = 0.012$, $A_1 = 3.60\text{x}10^{-2}$, $A_2 = 6.39\text{x}10^{-2}$ with a "goodness" calculated by Eq. 2 of $h(\xi) = 0.015$, the variance of the estimate log C. For comparison, the method of color index was applied to the entire simulated data set. The specific indexes used were $I_1 = L(443)/L(550)$ and $I_2 = L(520)/L(550)$. The method of least squares was used to obtain the goodness parameters, which for the two indexes chosen were 0.131 and 0.067 respectively. Additionally the method given by Sathyendranath, *et al.*, (1989) was applied to the data set. This method used the 5 wavelengths – 410, 445, 520, 565 and 640 nm – with a triangularly shaped spectral window of half-width 5 nm. The goodness or variance of the estimate using this method was 0.039. In summary, the goodness values, i.e., the variances of the estimate log C, were as follows: for Optimal Design, $h(\xi) = 0.015$; for the two color indexes, $h(\xi) = 0.131$ and 0.067; and for the method of Sathyendranath, *et al.*, 1989, $h(\xi) = 0.039$. Thus the Optimal Design method provided the highest retrieval accuracy of the methods considered.

5.0 TEST OF OPTIMAL DESIGN ROBUSTNESS

The computed ideal optimal design was tested for robustness and stability using more stringent conditions as follows: 1) The receiver related characteristic $M = A\,\omega\,t$ was taken to be 100 times smaller, and the detector noise used was 100 times greater than in basic model. 2) The solar angle range was extended to $\theta_0 = 30°$ to $70°$ rather than the range $\theta_0 = 40°$ to $60°$ in the basic model. This meant the working day was lengthened with observations made closer to dawn and dusk. 3) A narrower range of chlorophyll, sediment, and yellow substance concentrations were considered, i.e., $C = 0.02$ to 20 mg m^{-3}, $X = 0.02$ to 3 m^{-1}, $Y = 0.01$ to 1 m^{-1}. Additionally, per Kopelevich, *et al.*, (1994) a relation between C and Y was introduced where $Y = 0.427\,(-0.008 + 0.261C)$ when $C > 0.4$. And finally, 4) The Inherent Optical Property model (IOP) of Kopelevich, *et al.*, (1994) replaced the model of Sathyendranath, *et al.*, (1989) and Prieur, *et al.*, (1981).

Table 4 summarizes the resulting impact on chlorophyll estimation under the just mentioned parameter changes. The second column names the changed parameter. Each time a change was run, the resulting filter combinations and weights were slightly changed from the base case. The third column gives the new variance in

the log chlorophyll estimate with the new Optimal Design. The fourth column shows what variance would be if the filter combination and weights computed for the base sensor case were left unchanged. Note that for this case, Model number 0, the two variances are equal. Robustness is demonstrated by noting that even for extreme changes of input parameters different from the base case, the worst variance in the fourth column still only deviates by a factor of 1.8 from the new Optimal design. Even for this worst case the goodness or variance shown is still from 4 to 14 times better than that of the color index and principal component methods previously discussed.

Table 4. Variance of Estimate

Model Number	Parameters varied for robustness test	Variance of log Chlorophyll estimate	
		Changed OD	Baseline OD
0	Basic model	0.0099	0.0099
1	Sensor resource M	0.0114	0.0150
2	Range of solar angle θ_0	0.0110	0.0155
3	Range of concentrations X, Y, C	0.0096	0.0121
4	IOP model	0.0103	0.0188

6.0 CONCLUSIONS

For data gathered with remote optical spectral sensors, the optimal design algorithm gives a better estimate of chlorophyll (and/or other) concentrations than do the present methods of color index and principal component analysis. The Optimal Design method has been shown to be very robust to changes in experimental conditions and the models used to determine Inherent Optical Properties. The hyperspectral detector provides a simple realization of the OD algorithm with some sacrifice in retrieval accuracy because of finite spectral width. A limitation of this study, and hence of the resulting optimal designs, was that the radiance spectra used as the basis for the OD computations were simulated and not measured. Another limitation of the simulated data was that fluorescence and the sea bottom effects were not considered.

The next step in the solution of the problem should be an extensive collection of ocean radiance spectra with a hyperspectral sensor together with field truth measurements of the in situ optically active materials. This would provide an experimental basis for the comprehensive statistic ($u(\lambda)$, Θ) and allow the computation of a really optimal design. In the future we will apply the OD theory to the problem of bottom imagery. Additionally, we will tailor the sensor system and retrieval algorithm to match the water of the local area of interest and optimize the remote estimation of chlorophyll and other optically active oceanic parameters.

7.0 ACKNOWLEDGMENTS

This work was supported by the US Department of Defense under contract SP4700-96-M-0186, and by the Russian Foundation for Basic Research (RFBR), projects No 98-05-64983 and No. 98-05-65058.

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	October 1998	Professional Paper

4. TITLE AND SUBTITLE
Application of Experimental Design Theory to Ocean Remote Sensing With a Hyperspectral Detector

5. FUNDING NUMBERS
PR: SX08
PE: 0603714D
WU: DN305532
Contract No.: N66001-95-C-0055

6. AUTHOR(S)
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San Diego, CA 92152–5001

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Institute of Oceanology
St. Petersburg, Russia

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Office of the Secretary of Defense
Washington, DC 20301-8000

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENTR
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

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Published in "Proceedings of the Fifth International Conference on Remote Sensing for Marine and Coastal Environments," Vol. 1, pp. I-467-I-473, October 1998.

14. SUBJECT TERMS
Mission Area: Ocean Surveillance
Optical Detection — Physical Oceanography
Antisubmarine Warfare — Lasers

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	Same as Report

21a. NAME OF RESPONSIBLE INDIVIDUAL	21b. TELEPHONE *(include Area Code)*	21c. OFFICE SYMBOL
S. E. Stewart	(619) 553-2546	Code D743